1-Methyl-6-(2-methylphenyl)-1,6-dihydro-3-pyridinecarbonitrile 27531-42-6 | DTXSID60299776

	27301 42 0 01701000233770			
Model Performance				
<u>vioderi eriormance</u>				
NA - J - I	D.1.			
Model	Data			

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 3.11

Global applicability domain: Inside

Local applicability domain index: 5.76e-01

Confidence level: 7.57e-01

Nearest Neighbors from the Training Set

Image not found

1-Piperidineacetamide, N-(2-

bromophenyl)-Measured: 2.94 Predicted: 3.12

Image not found

1-Piperidineacetamide, N-(3-

chlorophenyl)-Measured: 3.45 Predicted: 3.22

Image not found

1-Piperidineacetamide, N-(3-

bromophenyl)-Measured: 3.62 Predicted: 3.13

Image not found

ST50451528 Measured: 3.57 Predicted: 3.13